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A perturbative approach for the crystal chains with self-consistent stochastic reservoirs

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Abstract We consider the harmonic chain of oscillators with self-consistent stochastic reservoirs and give a new proof for the finitude of its thermal conductivity in the steady state. The approach, with involves an integral representation for the correlations (heat flow) and a perturbative analysis, is quite general and extendable to the study of anharmonic systems.

Keywords Fourier's law · harmonic crystal · stochastic reservoirs

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In nonequilibrium statistical physics, the analytical derivation of the macroscopic laws of thermodynamics for microscopic models of interacting particles is a challenge to theorists. In particular, even in 1D context, it is still unknown the rigorous derivation of Fourier's law of heat conduction which states that the heat flow is proportional to the gradient of the temperature [1]. Many works, almost all of them by means of computer simulations [2] and with conflicting results have been devoted to the theme since the pioneering rigorous study on the harmonic chain of oscillators with thermal baths at the boundaries [3], a model that does not obey the Fourier's law. Recently, in the scenario of analytical studies, the harmonic chain of oscillators has been revisited, but in the case of each site coupled to a stochastic reservoir: it is

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proved that the Fourier's law holds in such case [4]; of course, if we turn off the coupling with the inner reservoirs, the heat conductivity diverges and the Fourier's law does not hold anymore, as previously shown in [3]. As the procedure presented in [4] was completely dependent on the linearity of the dynamics (i.e., on the harmonicity of the potential), some of the present authors have proposed a different approach to study the chain of oscillators with a reservoir at each site in order to analyze the problem of anharmonic potentials and infer their behavior with thermal baths at the boundaries only [5,6,7]. The proposed approach involves an integral representation for the correlations (related to the heat flow), whose analysis is carried out by means of a perturbative computation.

In the present letter, as a rigorous support for our previous theoretical works (which involve, as said, anharmonic interactions), we turn to the simpler case of the harmonic chain with a reservoir at each site and give a new proof for the finitude of the thermal conductivity (that shall be extendable to the anharmonic case), using our approach and a perturbative analysis: the expression for the conductivity presented here coincide with that one described in [4].

Let us introduce the model. We consider a lattice system with unbounded scalar variables in a space $\Lambda \subset \mathbb{Z}$ and with stochastic heat bath at each site. Precisely, we take a system of N oscillators with the Hamiltonian

$$H(p, q) = \sum_{j=1}^N \frac{1}{2} (p_j^2 + M q_j^2) + \frac{1}{2} \sum_{j \neq l=1}^N q_j J_{jl} q_l, \quad (1)$$

where $J_{lj} = J_{jl}$ and $J_{lj} = f(|l - j|)$. In the study of harmonic chains it is usually taken j and l nearest neighbors and $J_{j,j+1} = J$ for any j . In this case, the interparticle interactions may be also written as (assuming Dirichlet boundary conditions $q_0 = 0 = q_{N+1}$)

$$\sum_{j=1}^N V(q_j - q_{j+1}) \quad , \quad V = \frac{J^2}{2} q^2, \quad (2)$$

after adjustments in M , the coefficient of q_j^2 . We consider the Langevin time evolution given by the stochastic differential equations

$$\begin{aligned} dq_j &= p_j dt, \\ dp_j &= -\frac{\partial H}{\partial q_j} dt - \xi p_j dt + \gamma_j^{1/2} dB_j, \quad j = 1, 2, \dots, N, \end{aligned} \quad (3)$$

where B_j are independent Wiener processes (i.e., $\eta_j = dB_j/dt$ are independent white noises) ξ is the coupling between the site j and its heat bath; $\gamma_j \equiv 2\xi T_j$, where T_j is the temperature of the j -th reservoir. As usual, we define the energy of a single oscillator as

$$H_j(q, p) = \frac{1}{2} p_j^2 + q_j^2 + U(q_j) + \frac{1}{2} \sum_{l \neq j} V(q_j - q_l), \quad (4)$$

where the expressions for U and V follow from eq. (1) and from $\sum_j H_j = H$. Then for the energy current we have

$$\left\langle \frac{dH_j}{dt} \right\rangle = \langle R_j \rangle - \langle \mathcal{F}_{j\leftarrow} - \mathcal{F}_{j\rightarrow} \rangle, \quad (5)$$

where $\langle \cdot \rangle$ means the expectation with respect to the noise distribution; R_j denotes the energy flux between the j -th reservoir and the j -th site

$$\langle R_j \rangle = \xi (T_j - \langle p_j^2 \rangle); \quad (6)$$

and the energy current in the chain is

$$\begin{aligned} \mathcal{F}_{j\rightarrow} &= \sum_{l>j} \nabla V(q_j - q_l) \frac{p_j + p_l}{2}, \\ \mathcal{F}_{j\leftarrow} &= \sum_{l<j} \nabla V(q_l - q_j) \frac{p_l + p_j}{2}. \end{aligned} \quad (7)$$

As well known, the stationary state is characterized by $\langle dH_i/dt \rangle = 0$; and, for physical reasons, it is interesting to consider the “self-consistent condition” given by $\langle R_j \rangle = 0$ in the steady state. For the linear dynamics, the existence and convergence to the stationary state as $t \rightarrow \infty$ are old solved problems, see e.g. [8].

Lets us state our main theorem.

Theorem 1 *For the harmonic chain of oscillators with reservoirs at each site (1-3), in the case of nearest neighbor interactions, i.e. $J_{jl} = J(\delta_{l,j+1} + \delta_{l,j-1})$, with $J < J_0$ for some small J_0 , the Fourier’s law holds*

$$\mathcal{F} = \lim_{t \rightarrow \infty} \langle \mathcal{F}_{j\rightarrow} \rangle = -\frac{\chi}{N-1} (T_N - T_1), \quad (8)$$

with the “self consistent” condition $\lim_{t \rightarrow \infty} \langle R_j \rangle = 0$ for the inner sites j , and with the heat conductivity χ given by

$$\chi = \frac{J^2}{2\xi M} + \mathcal{O}(J^3). \quad (9)$$

Remark 1 A theorem establishing the finitude of the thermal conductivity for the considered model has been already presented in [4], as already said, and with the nearest neighbor interparticle potential not necessarily small. Our aim in this letter, as emphasized, is not to give a second proof but to present a more general approach which shall extend to the anharmonic chains.

Remark 2 Following the steps to be presented ahead, we may also study the heat flow for weak interparticle interactions beyond nearest neighbor: e.g. for $\sup_l \sum_j J_{lj} \leq J_0$.

Now we describe our approach. It is usefull to introduce the phase-space vector $\phi = (q, p)$ and write the dynamics as

$$\dot{\phi} = -A\phi + \sigma\eta, \quad (10)$$

where $A = A^0 + \mathcal{J}$ and σ are $2N \times 2N$ matrices

$$A^0 = \begin{pmatrix} 0 & -I \\ \mathcal{M} & \Gamma \end{pmatrix}, \mathcal{J} = \begin{pmatrix} 0 & 0 \\ \mathbb{J} & 0 \end{pmatrix}, \sigma = \begin{pmatrix} 0 & 0 \\ 0 & \sqrt{2\Gamma\mathcal{T}} \end{pmatrix}, \quad (11)$$

where I is the unit $N \times N$ matrix, \mathbb{J} is the $N \times N$ matrix for the interparticle interactions, and \mathcal{M} , Γ and \mathcal{T} are the diagonal $N \times N$ matrices: $M_{jl} = M\delta_{jl}$, $\Gamma_{jl} = \xi\delta_{jl}$, $\mathcal{T} = T_j\delta_{jl}$. And η are independent white noises. In what follows we will use the index notation: i for index values in the set $[N+1, N+2, \dots, 2N]$; j for values in the set $[1, 2, \dots, N]$ and k for values in $[1, 2, \dots, 2N]$. We will also omit obvious sums over repeated indices.

Our strategy is first to consider (10) above with $\mathcal{J} \equiv 0$, i.e., a system with isolated sites (without interactions among them). In a second step we introduce the interparticle interaction by using the Girsanov theorem, and then we calculate the heat flow in a perturbative computation.

We have

Lemma 1 *The solution of (10) with $\mathcal{J} \equiv 0$ is the Ornstein-Uhlenbeck Gaussian process*

$$\phi(t) = e^{-tA^0}\phi(0) + \int_0^t ds e^{-(t-s)A^0}\sigma\eta(s), \quad (12)$$

where, for the simple case of $\phi(0) = 0$, the covariance of the process evolves as

$$\langle \phi(t)\phi(s) \rangle_0 \equiv \mathcal{C}(t, s) = \begin{cases} e^{-(t-s)A^0}\mathcal{C}(s, s), & t \geq s, \\ \mathcal{C}(t, t)e^{-(s-t)A^{0\top}}, & t \leq s, \end{cases} \quad (13)$$

$$\mathcal{C}(t, t) = \int_0^t ds e^{-sA^0}\sigma^2 e^{-sA^{0\top}}. \quad (14)$$

Proof It is a simple exercise of stochastic differential equations (see e.g. [9], p.74) \square .

In the simple case of $\mathcal{J} \equiv 0$, as $t \rightarrow \infty$ we have a convergence to the Gaussian distribution with covariance

$$C = \int_0^\infty ds e^{-sA^0}\sigma^2 e^{-sA^{0\top}} = \begin{pmatrix} \frac{\mathcal{T}}{\mathcal{M}} & 0 \\ 0 & \mathcal{T} \end{pmatrix}, \quad (15)$$

where as said, \mathcal{T} is a diagonal $N \times N$ matrix with $\mathcal{T}_{ij} = T_i\delta_{ij}$ (see e.g. [8]).

The solution of (10) with the interparticle potential will be derived from the particular case of $\mathcal{J} \equiv 0$ by using the Girsanov theorem which establishes a measure ρ for the complete process in terms of the measure μ_C obtained for $\mathcal{J} \equiv 0$. Precisely, for the two-point function we have

Lemma 2 *The two-point functions for the complete process (10) can be written as*

$$\langle \varphi_u(t_1) \varphi_m(t_2) \rangle = \int \phi_u(t_1) \phi_m(t_2) Z(t) d\mu_C / \text{norm.}, \quad t_1, t_2 < t, \quad (16)$$

where ϕ is the solution (given by Lemma 1) of the process with $\mathcal{J} \equiv 0$, and φ is the solution for the complete process (10). \mathcal{C} is given by (13,14), and the corrective factor is

$$Z(t) = \exp \left(\int_0^t u \cdot dB - \frac{1}{2} \int_0^t u^2 ds \right), \quad (17)$$

$$\gamma_i^{1/2} u_i = -J_{i-N,j} \phi_j.$$

Proof For the harmonic potential, the process is an Itô diffusion, and so, the proof is also direct: see e.g. theorem 8.6.8 in [9]. \square

Remark 3 In the case of the nonlinear (anharmonic) dynamical system problem we may introduce the anharmonic interactions (on-site and/or interparticle potentials) still by using the Girsanov theorem: e.g., for bounded potentials or initial processes with continuous realization, the use of Novikov condition makes the procedure straightforward; see an example of other manipulations in a similar use of the Girsanov theorem [10].

Turning to the $Z(t)$ expression above, we have

$$\begin{aligned} u_i dB_i &= \gamma_i^{-1/2} u_i \gamma_i^{1/2} dB_i \\ &= \gamma_i^{-1/2} u_i (d\phi_i + A_{ik}^0 \phi_k dt) \\ &= -\gamma_i^{-1/2} \mathcal{J}_{ij} \phi_j (d\phi_i + A_{ik}^0 \phi_k dt). \end{aligned} \quad (18)$$

Using the Itô formula we get

$$\begin{aligned} -\gamma_i^{-1} \mathcal{J}_{ij} \phi_j d\phi_i &= -dF - \gamma_i^{-1} \phi_i \mathcal{J}_{ij} A_{jk}^0 \phi_k dt, \\ F(\phi) &= \gamma_i^{-1} \phi_i \mathcal{J}_{ij} \phi_j. \end{aligned} \quad (19)$$

And so,

$$Z(t) = \exp \left(\int_0^t u \cdot dB - \frac{1}{2} \int_0^t u^2 ds \right) \quad (20)$$

$$= \exp [-F(\phi(t)) + F(\phi(0))] \exp \left[- \int_0^t W(\phi(s)) ds \right],$$

$$\begin{aligned} W(\phi(s)) &= \gamma_i^{-1} \phi_i(s) \mathcal{J}_{ij} A_{jk}^0 \phi_k(s) + \phi_k(s) A_{ki}^{0\top} \gamma_i^{-1} \mathcal{J}_{ij} \phi_j + \\ &+ \frac{1}{2} \phi_{j'}(s) \mathcal{J}_{j'i} \gamma_i^{-1} \mathcal{J}_{ij} \phi_j(s). \end{aligned} \quad (21)$$

To analyze the heat flow in the steady state (related to $\lim_{t \rightarrow \infty} \langle \varphi_u(t) \varphi_v(t) \rangle$), we note that we may write

$$\exp(-tA^0) = e^{-t\frac{\xi}{2}} \cosh(t\rho) \left\{ \begin{pmatrix} I & 0 \\ 0 & I \end{pmatrix} + \frac{\tanh(t\rho)}{\rho} \begin{pmatrix} \frac{\xi}{2} & I \\ -\mathcal{M} & -\frac{\xi}{2} \end{pmatrix} \right\}, \quad (22)$$

$\rho = \left(\left(\frac{\xi}{2} \right)^2 - M \right)^{1/2}$. It may be shown by e.g., diagonalizing A^0 (or see the appendix of [4]). We also note that

$$\mathcal{C}(t, s) = \exp(-(t-s)A^0) C + \mathcal{O}(\exp(-(t+s)\xi/2)), \quad (23)$$

where the effects in the correlation function formula of the second term on the right-hand side of the equation above vanishes in the limit $t \rightarrow \infty$; C is the covariance (15).

Now, to compute the two-point correlation function (16) (and so, the heat flow), we expand the exponential which gives $Z(t)$ above (20-21) in a power series: $\exp[X] = \sum_{n=0}^{\infty} X^n/n!$, and calculate the connected Feynman graphs for (16) (due to the normalization factor we stay with the connected graphs only) using the Wick theorem. As we have quadratic terms in ϕ in the exponent (see F and W above), there is no countable problem with the series; roughly,

$$\left| \int \frac{\phi^{2n}}{n!} d\mu_C \right| = \left| \frac{1}{n!} \sum_{k=1}^{(2n-1)!!} \underbrace{(\mathcal{C}\mathcal{C}\cdots\mathcal{C})}_n \right| \leq \frac{(2n)!!}{n!} |\mathcal{C}\cdots\mathcal{C}| = 2^n |\mathcal{C}\cdots\mathcal{C}|. \quad (24)$$

In short, to control the expansion we only need a bound for the n convolutions of the covariance \mathcal{C} such as $c^n J^n$, where c is some constant. Thus at least for small J , this simple analysis will give us the convergence of the perturbative series. To get such bound, we use the formulas (22-23) for \mathcal{C} , the lemma below and that

$$\begin{aligned} \|C\| &\leq c_1(1 - e^{-2\alpha t}), \\ \|e^{-tA^0}\| &\leq c_2 e^{-\alpha t}, \\ \|A^0\| &\leq c_3, \end{aligned}$$

where $\alpha = \min\{\xi/2, M/\xi\}$ ($\|\bullet\|$ means a matrix bound on $M_{2N \times 2N}(\mathbb{R})$).

Lemma 3 *Let I_t be*

$$I_t = \int_0^t e^{-\alpha|t-s_1|} e^{-\alpha|s_1-s_2|} \cdots e^{-\alpha|t-s_n|} ds_1 \cdots ds_n, \quad \alpha > 0, \quad (25)$$

then, $\lim_{t \rightarrow \infty} I_t \leq (c_\alpha)^n$, where c_α does not depend on n .

Proof For $f(x) = e^{-\alpha|x|}$, we have

$$\tilde{f}(p) \equiv \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-ipx} e^{-\alpha|x|} dx = \frac{1}{\sqrt{2\pi}} \frac{2\alpha}{\alpha^2 + p^2}. \quad (26)$$

And

$$\begin{aligned}
I_t &\leq \frac{1}{2} \int_{-\infty}^{\infty} e^{-\alpha|t-s_1|} e^{-\alpha|s_1-s_2|} \dots e^{-\alpha|t-s_n|} ds_1 \dots ds_n \\
&= \frac{1}{2} \int_{-\infty}^{\infty} f(t-s_1) f(s_1-s_2) \dots f(s_n-t) ds_1 \dots ds_n \\
&= \frac{1}{2} \underbrace{f * f * \dots * f}_{n+1}(0) \\
&= \frac{1}{2} (2\pi)^{(n-1)/2} \int_{-\infty}^{\infty} (\tilde{f}(p))^{n+1} dp,
\end{aligned} \tag{27}$$

where $*$ means the convolution, and we have used Parseval's theorem in the last equality above. Hence,

$$\lim_{t \rightarrow \infty} I_t \leq \frac{1}{2} (2\pi)^{(n-1)/2} \int_{-\infty}^{\infty} \frac{1}{(2\pi)^{(n+1)/2}} \left(\frac{2\alpha}{\alpha^2 + p^2} \right)^{n+1} dp \leq (c_\alpha)^n. \tag{28}$$

Thus, using the formulas (22-23) for the covariance and the lemma 3 above, we may bound the terms order J^2 and up in the two point function (16) by

$$\sum_{n=2}^{\infty} (c' J)^n \leq c'' J^2, \tag{29}$$

where c' and c'' are some constants (i.e., they do not depend on n).

To obtain the result of theorem 1 we still need to calculate, in detail, the two-point correlation function up to first order in J . Carrying out the computation (simple Gaussian integrations), for $\langle \varphi_u \varphi_v \rangle \equiv \lim_{t \rightarrow \infty} \langle \varphi_u(t) \varphi_v(t) \rangle$, we obtain

$$\langle \varphi_u \varphi_v \rangle = \begin{cases} \frac{1}{2\xi M} [\mathcal{J}_{v+N, u-N} T_{u-N} - \mathcal{J}_{u, v} T_v], & \text{for } \begin{cases} u \in [N+1, \dots, 2N], \\ v \in [1, \dots, N], \end{cases} \\ T_{u-N} \delta_{u, v}, & \text{for } u, v \in [N+1, \dots, 2N]. \end{cases} \tag{30}$$

Hence, from (7)

$$\mathcal{F}_{j \rightarrow} = \sum_{r > j} \mathcal{J}_{j+N, r} (\varphi_j - \varphi_r) \frac{(\varphi_{j+N} + \varphi_{r+N})}{2}, \quad r \in [1, \dots, N], \tag{31}$$

and we have (for $\langle \varphi_u \varphi_v \rangle$ up to first order in J)

$$\langle \mathcal{F}_{j \rightarrow} \rangle = \sum_{r > j} \frac{(\mathcal{J}_{j+N, r})^2}{2\xi M} (T_r - T_j), \tag{32}$$

or, for nearest neighbor interactions,

$$\mathcal{F}_{j \rightarrow j+1} = \langle \mathcal{F}_{j \rightarrow} \rangle = \frac{(\mathcal{J}_{j+N, j+1})^2}{2\xi M} (T_{j+1} - T_j). \tag{33}$$

The first order perturbation computation (30) above still gives us

$$\lim_{t \rightarrow \infty} \langle R_j(t) \rangle = 0.$$

Thus, the steady state condition $\langle dH_i/dt \rangle = 0$ leads to

$$\mathcal{F}_{1 \rightarrow 2} = \mathcal{F}_{2 \rightarrow 3} = \dots = \mathcal{F}_{N-1 \rightarrow N} \equiv \mathcal{F}. \quad (34)$$

And so, for the simpler case of the same interactions between any two nearest neighbors sites, i.e., $J = \mathcal{J}_{j+N,j+1}$ for any j , it follows that (for $\langle \varphi_u \varphi_v \rangle$ up to first order in J), we have

$$\mathcal{F}_{\rightarrow} = \chi \frac{T_N - T_1}{N - 1}, \quad \chi = \frac{J^2}{2\xi M}. \quad (35)$$

From (31) and (29), it is easy to see that considering the remaining terms (higher order in J), we get as $J \times cJ^2 = cJ^3$ in χ (the temperature terms $T_{j+1} - T_j$ may be extract from the perturbative analysis following the products of C , the covariance (15) in \mathcal{C} which appears in the Gaussian interaction, and the terms γ_i coming from the expansion of $Z(t)$). In short, theorem 1 holds.

Remark 4 In the case of anharmonic terms in W and F (19-21), a naive expansion fails, but we expect to develop a perturbative approach by using some cluster expansion as well known in field theory and statistical mechanics. For the simpler case of nonconservative nonlinear stochastic dynamical model (describing a system in contact with thermal reservoirs at the same temperature, and so going to equilibrium), a convergent cluster expansion is presented in [10], and the decay of the four-point function is investigated in [12] and [11]: the complete and rigorous result [11] adds only small corrections to the first order perturbative calculation [12].

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